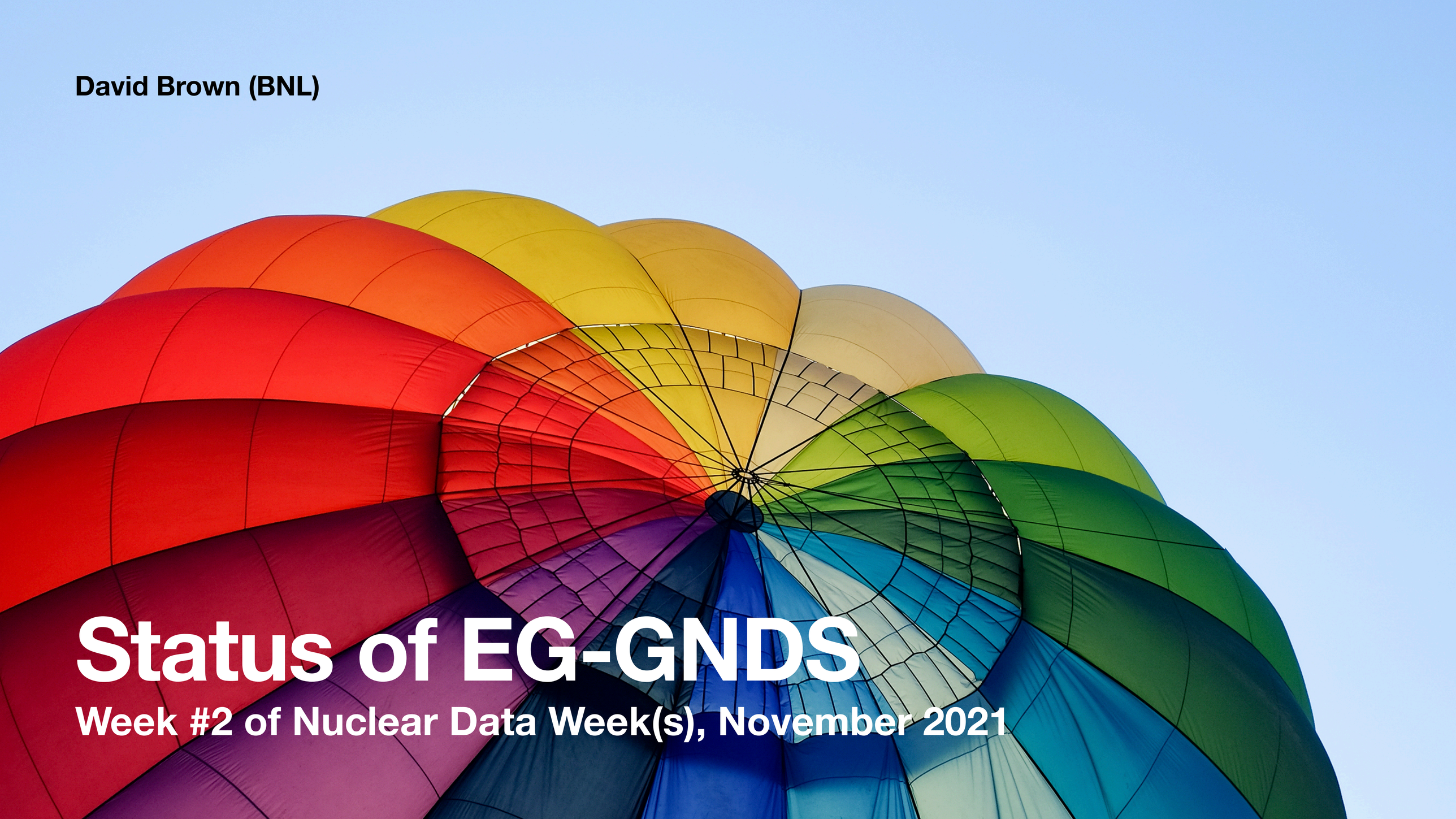
David Brown (BNL)

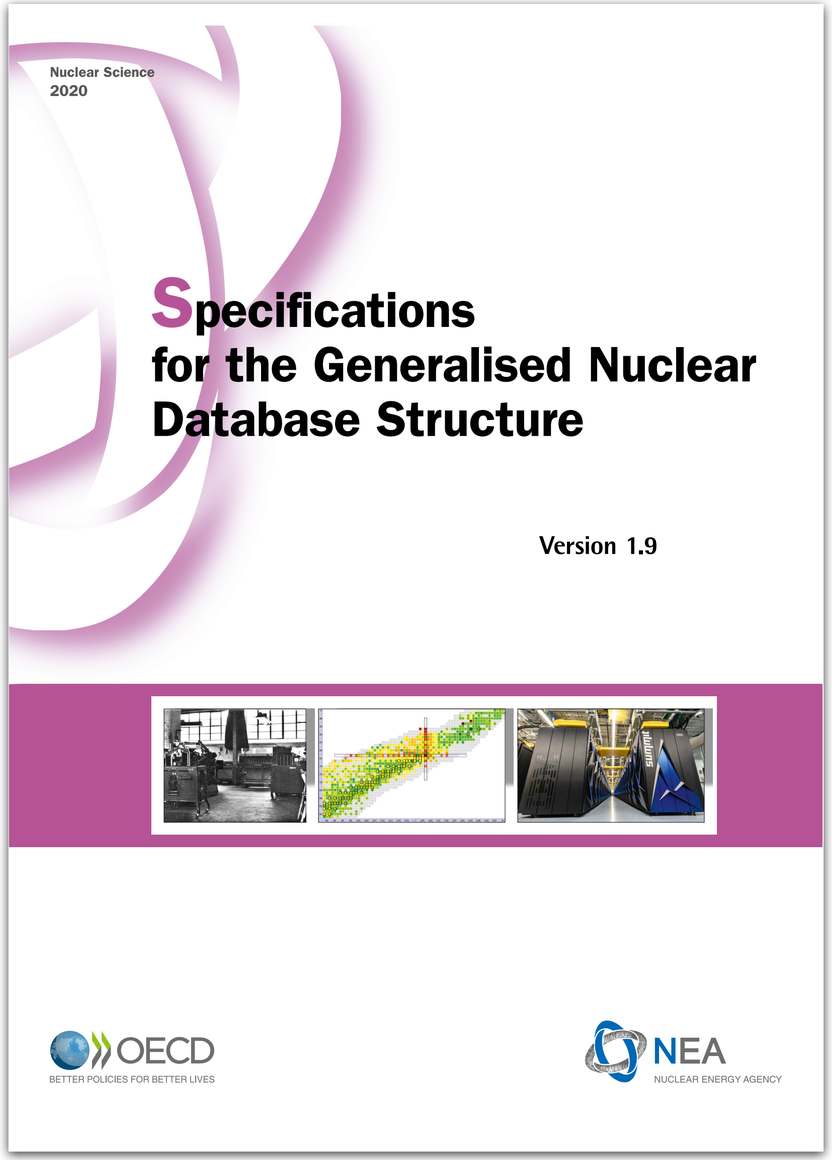


Status of EG-GNDS

Week #2 of Nuclear Data Week(s), November 2021

GNDS-1.9 specifications published Summer 2020

- Specifications: https://oecd-nea.org/download/wpec/documents/7519-GNDS.pdf
- XML Schema for GNDS-1.9: https://www.oecd-nea.org/download/wpec/gnds/gnds.xsd
- GNDS Webinar: https://www.youtube.com/watch?v=h9Byrkxr8LE&feature=youtu.be

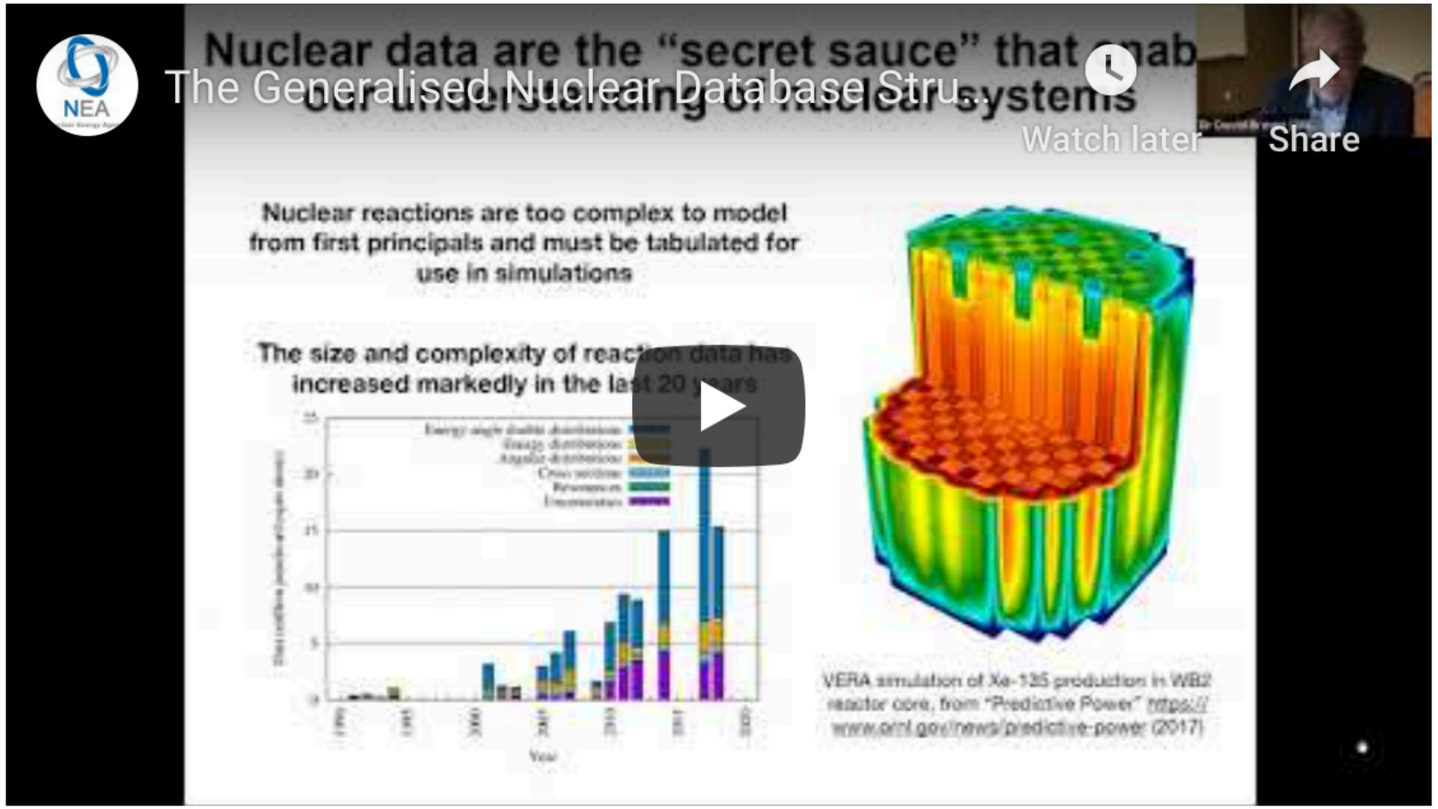


Thank you webinar participants

https://www.youtube.com/watch?v=h9Byrkxr8LE&feature=youtu.be

The NEA hosted an expert roundtable webinar on GNDS on 8 July 2020. The discussion was be moderated by William D. Magwood, IV, NEA Director-General and Dr David Brown (BNL), Chair of the NEA Expert Group on the Recommended Definition of a General Nuclear Database Structure (GNDS). The panellists included:

- Dr Osamu Iwamoto (JAEA)
- Dr Jean-Christophe Sublet (IAEA)
- Dr Dorothea Wiarda (ORNL)
- Dr Caleb Mattoon (LLNL)
- Dr Fausto Malvagi (CEA)



Meetings/events since GNDS-1.9 approved

- **June 2019:** 31st WPEC - approved, figured out improvement process, made 2.0 branch - *last in person meeting*
- **May 2020:** 32nd WPEC - progress on 2.0
- **July 2020:** GNDS-1.9 Published
- **July 2020:** GNDS-1.9 Webinar
- **Dec. 2020:** Nuclear Data Week 2020 - status report
- **9-10 Nov 2020:** WPEC SG meeting - progress on 2.0
- **May 2021:** 33rd WPEC - final feature freeze, except for resonance issues
- **Aug. 2021:** mini-CSEWG - status report
- **20 Oct. 2021:** EG-GNDS Meeting - final approval on most open trackers
- **Nov. 2021:** Nuclear Data Weeks(s) 2021 - *now*

- **Dec. 2021:** Anticipate approval @ WPEC meeting, editing process begins
- **May 2022**: 34th WPEC - planned announcement of GNDS-2.0

What did we do the last two or so years?

GNDS-2.0 Highlights

- **xsdir-like functionality:**
  `map` file and `checksum` support
- **Documentation markup:**
  supports all metadata needed for DataCite.org DOI assignment
- **Ground-up rewrite of TNSL**
  - In collaboration with SG-42,48
  - Mixed elastic scattering
  - TNSL covariance
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```
<map library="neutrons" format="0.2"
        checksum="c180fbca8661de7e053ddbe1a7101ac371e79428" algorithm="sha1">
  <protare projectile="n" target="H1" evaluation="ENDF/B-8.0"
        path="n-001_H_001.xml" interaction="nuclear"
        checksum="32518f6f6ec82c801531ae120618bd99d3589304"/>
  <TNSL projectile="n" target="HinCH2" evaluation="ENDF/B-8.0"
        path="tsl-HinCH2.xml"
        checksum="dea956df66b3cef44d690efba983d537dca0a997"
        standardTarget="H1" standardEvaluation="ENDF/B-8.0"/>
  <protare projectile="n" target="O16" evaluation="ENDF/B-7.1"
        path="n-008_O_016.xml" interaction="nuclear"
        checksum="ff118f6851181c244e494921c6e56101dabf6200"/>
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        path="n-013_Al_027.xml" interaction="nuclear"
        checksum="c3bd9de97a51a5a7c05489a3b5134bd02719942d"/>
                "n" target="tnsl-Al27" evaluation="ENDF/B-8.0"
                13_Al_027.xml"
                38572faa8fb763418a19b1a20d84165b02bdbe4"
                get="Al27" standardEvaluation="ENDF/B-8.0"/>
                le="n" target="Fe56" evaluation="ENDF/B-7.1"
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                3ab2d67e59d5a8bb5820cafe67a0b8d498f0870"/>
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        path="n-090_Th_227.xml" interaction="nuclear"
        checksum="1dca182331b2d482d2dfa6d7142f1a36fc833dd9"/>
</map>
```
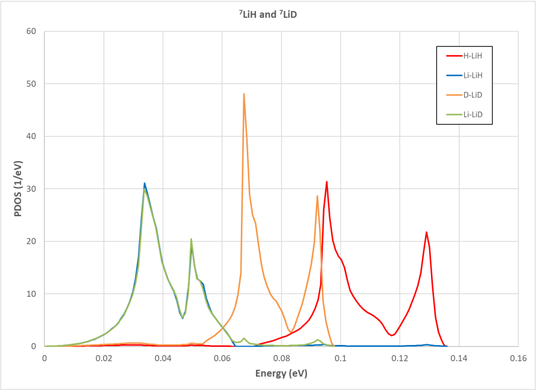
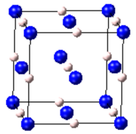
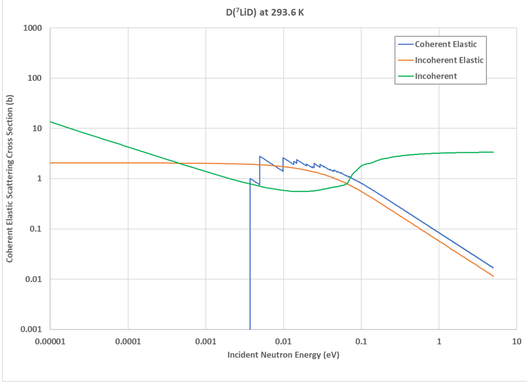





LiH unit cell
(4.0831 Å for LiH,
4.0684 Å for LiD)



Map file -- test.map

```
<map library=”test22" format="0.2">

<protare projectile="n"  target=”O16"  evaluation=”fromJoe”
                          path=”fromJoe/n-008_O_016.xml"/>
<protare projectile="n"  target=”U235"  evaluation=”fromJoe”
                          path=”fromJoe/n-092_U_235.xml"/>

<protare projectile="n"  target=”U235"  evaluation=”Ian”
                          path=”fromIan/n-092_U_235.xml"/>
<protare projectile="n"  target=”U238"  evaluation=”Ian”
                          path=”fromIan/n-092_U_238.xml"/>

<TNSL projectile="n"  target="OinBeO"  evaluation="ENDF/B-8.0”
                          path="tsl/tsl-OinBeO.xml">
                          standardTarget="O16" standardEvaluation="ENDF/B-8.0”/>

<import production.map></map>
```

C. Mattoon, WPEC May 2021

New multi-group boundaries and flux file

- Multi-group boundaries format uses GNDS <group> node to store the label and boundaries for a group.

```
<group label="LLNL_gid_23">
  <grid index="0" label="energy" unit="MeV" style="boundaries">
   <values>2.0908e-6 2.0908e-4 1.8817e-3 .010245 .07002 0.27097 .7527 15.754</values></grid></group>
```

- Flux stored as f(T,E,mu) using a GNDS 3d function.

```
<XYs3d label="LLNL_fid_1">
  <axes>
   <axis index="3" label="temperature" unit="MeV/k"/>
   <axis index="2" label="energy_in" unit="MeV"/>
   <axis index="1" label="mu" unit=""/>
   <axis index="0" label="flux" unit="1/s"/></axes>
  <XYs2d outerDomainValue="0.0">
   <Legendre outerDomainValue="0.0"><values>85</values></Legendre>
   <Legendre outerDomainValue="21.0"><values>85</values></Legendre></XYs2d></XYs3d>
```

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                38572faa8fb763418a19b1a20d84165b02bdbe4"
                get="Al27" standardEvaluation="ENDF/B-8.0"/>
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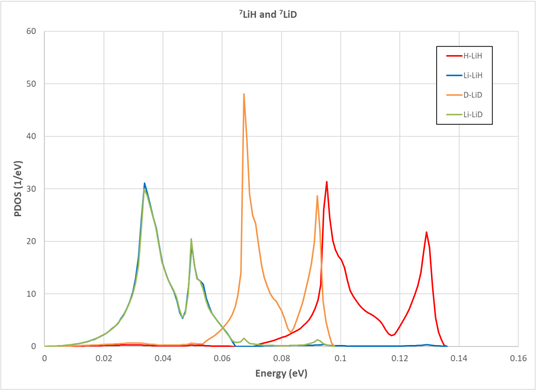
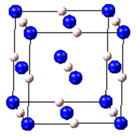
</map>
```





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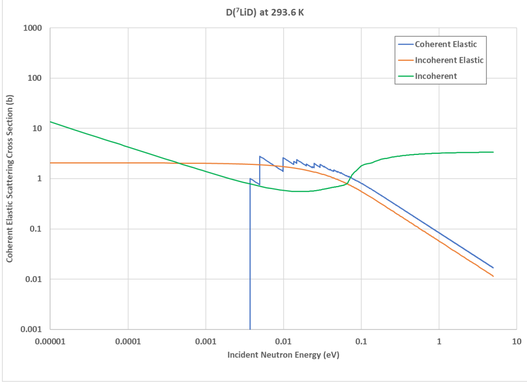

Metadata requires a longer discussion

- **There are 4 sources of metadata schema between OSTI and DataCite.org**

Many of the markups are being adopted(adapted?) for GNDS-2.0

- authorship vs. contributor - give proper credit for level of work
- dates - much broader set of events than ENDATE, RDATE, DDATE and EDATE
- relationship - which set is related to what other set and how

I believe adopting these markups in GNDS and the metadata schema can relieve many stressors within CSEWG!

Problem #1: Giving credit where credit is due

PROBLEM

- **The ENDF-6 format does not have enough space for all the authors**
  - Overflow must be listed in free-text fields with unclear rules both for credit and formatting
- **The ENDF-6 format does not have scheme for denoting smaller (but still important) contributions**
  - These must be listed in free-text fields with unclear rules both for credit and formatting

SOLUTION (PARTIAL)

- **Assigning proper credit:**
  - <authors> - list of authors & affiliations of whatever length is needed
- **Capturing minor changes:**
  - <contributors> - list of contributors with nature of contribution ()
  - <dates> - list of dates with nature of data ()

D. Brown, mini-CSEWG, Aug. 2021

ENDF Discussion: What Criteria Elevates a Contributor to an Author? What is the order for Authors?
(My thoughts below)

- Bug fixes -> Contributor
  - Includes fixing normalizations, threshold energies, typos,
- Major changes to evaluation -> Author
- Lead author/Creator/PI -> Authors plz figure it out

- Lead author should be negotiated by the authors and the CSEWG executive committee if it is not clear or if there is disagreement
- Order of authors should be handled in similar manner

Problem #2: Meager explanation of versioning within an ENDF file

PROBLEM

Within an ENDF file, changes denoted with ENDATE, NMOD and the dictionary

- We very rarely remember to change them
- Most of us don't know how to use them correctly

SOLUTION (PARTIAL)

<dates> markup lets us denote important dates in an evaluations lifecycle

- DataCite defines many useful dateTypes: accepted, available, submitted, updated, etc.
- <date dateType="accepted">…</date>

```
Merge IAEA-CRP PFNS with ENDF/B-VIII.0 for U-233                    7000 0  0    0
 9.223300+4 2.310380+2          1          1          0          19222 1451    1
 0.000000+0 1.000000+0          0          0          0          69222 1451    2
 1.000000+0 2.000000+7          0          0         10          89222 1451    3
 0.00000+00 0.00000+00          0          0        807        1369222 1451    4
 92-U -233 JAEA+      EVAL-JAN10 O.Iwamoto,N.Otuka,S.Chiba,et al. 9222 1451    5
 NDS 148, 1 (2018)    DIST-FEB18                       20100326   9222 1451    6
----ENDF/B-VIII.0     MATERIAL 9222                                9222 1451    7
-----INCIDENT NEUTRON DATA                                         9222 1451    8
------ENDF-6 FORMAT                                                9222 1451    9
                                                                   9222 1451   10
Resonance bound levels tuned to thermal const. of Standards-2017   9222 1451   11
```

```
                                                                   9222 1451  807
                                                                   9222 1451  808
                                                                   9222 1451  809
                                                                   9222 1451  810
 **************** Program DICTIN (VERSION 2018-1) ****************9222 1451  811
                                1        451        947          19222 1451  812
                                1        452         21          19222 1451  813
                                1        455          8          19222 1451  814
                                1        456         19          19222 1451  815
                                1        458          5          19222 1451  816
                                2        151        983          19222 1451  817
                                3          1         55          19222 1451  818
                                3          2         55          19222 1451  819
                                3          4         35          19222 1451  820
                                3         16         13          19222 1451  821
                                3         17          8          19222 1451  822
                                3         18         52          19222 1451  823
                                3         19         46          19222 1451  824
                                3         20         22          19222 1451  825
                                3         21         15          19222 1451  826
                                3         37          4          19222 1451  827
                                3         38          7          19222 1451  828
                                3         51         35          19222 1451  829
                                3         52         34          19222 1451  830
                                3         53         32          19222 1451  831
                                3         54         32          19222 1451  832
                                3         55         31          19222 1451  833
```

D. Brown, mini-CSEWG, Aug. 2021

Brookhaven National Laboratory

Problem #3: How sets are related to one another?

PROBLEM

The ENDF-6 format does not denote which file is derived from another. LDRV just flags that a file is derived.

GNDS provides evaluated and derived styles and a "derivedFrom" link. This solves the problem within a GNDS file.

How do I denote the ENDF->GNDS connection? The ENDF->ACE connection?

SOLUTION (PARTIAL)

<relatedItem name="..." href="..." relationType="…"/>

DataCite defines the following relationTypes:
'IsCitedBy','Cites','IsSupplementTo', 'IsSupplementedBy','IsContinuedBy', 'Continues', 'Describes', 'IsDescribedBy', 'HasMetadata', 'IsMetadataFor', 'HasVersion', 'IsVersionOf', 'IsNewVersionOf', 'IsPreviousVersionOf', 'IsPartOf', 'HasPart', 'IsPublishedIn', 'IsReferencedBy', 'References', 'IsDocumentedBy', 'Documents', 'IsCompiledBy', 'Complies', 'IsVariantFormOf', 'IsOriginalFormOf', 'IsIdenticalTo', 'IsReviewedBy', 'Reviews', 'IsDerivedFrom', 'IsSourceOf', 'IsRequiredBy', 'Requires', 'Obsoletes', 'IsObsoletedBy'

D. Brown, mini-CSEWG, Aug. 2021

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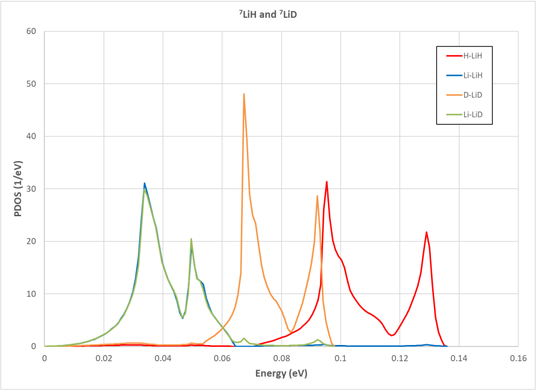

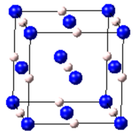

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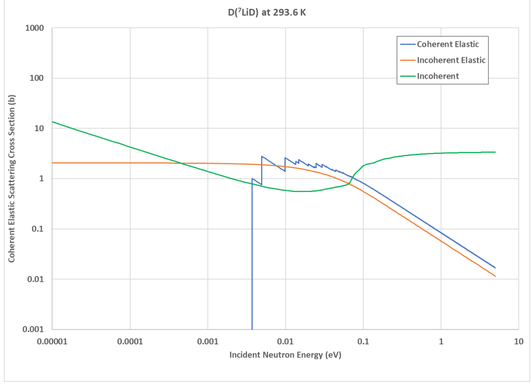


The hierarchy for storing TNSL data was overhauled between GNDS-1.9 and GNDS-2.0

GNDS-1.9

```
–<thermalScattering material="13-Al- 27" MAT="53">
  +<documentation name="endfDoc"></documentation>
   <cutoffEnergy value="5.0" unit="eV"/>
   <mass value="26.74975" unit="amu"/>
  –<coherentElastic>
    –<S_table>
      +<gridded2d label="eval"></gridded2d>
     </S_table>
   </coherentElastic>
  –<incoherentInelastic calculatedAtThermal="true">
    +<scatteringAtoms></scatteringAtoms>
    –<S_alpha_beta>
      +<gridded3d label="eval"></gridded3d>
     </S_alpha_beta>
   </incoherentInelastic>
 </thermalScattering>
```

GNDS-2.0

```
–<reactionSuite projectile="n" target="tnsl-Al27" evaluation="ENDF/B-8.0" format="1.10" projectileFrame="lab" interaction="TNSL">
  +<styles></styles>
  +<documentations></documentations>
  +<PoPs name="protare_internal" version="1.0" format="0.1"></PoPs>
  –<reactions>
    –<reaction label="n [thermalNeutronScatteringLaw coherent-elastic]" ENDF_MT="2">
      –<doubleDifferentialCrossSection>
        –<thermalNeutronScatteringLaw_coherentElastic label="eval" pid="n" productFrame="lab">
          –<S_table>
            +<gridded2d></gridded2d>
           </S_table>
         </thermalNeutronScatteringLaw_coherentElastic>
       </doubleDifferentialCrossSection>
      +<crossSection></crossSection>
      +<outputChannel genre="twoBody" process="thermalNeutronScatteringLaw coherent-elastic"></outputChannel>
     </reaction>
    –<reaction label="n [thermalNeutronScatteringLaw incoherent-inelastic]" ENDF_MT="4">
      –<doubleDifferentialCrossSection>
        –<thermalNeutronScatteringLaw_incoherentInelastic label="eval" pid="n" productFrame="lab">
           <options calculatedAtThermal="true" asymmetric="false"/>
          +<scatteringAtoms></scatteringAtoms>
          –<S_alpha_beta>
            +<gridded3d></gridded3d>
           </S_alpha_beta>
```

GNDS-2.0 layout integrates TNSL with all other reactions. Integrating and renormalizing TNSL double-differential cross sections produces a standard cross section and outgoing neutron distribution.

```
tic"></outputChannel>
 </reactionSuite>
```

C. Mattoon IAEA CM on Data Processing, Oct. 2021

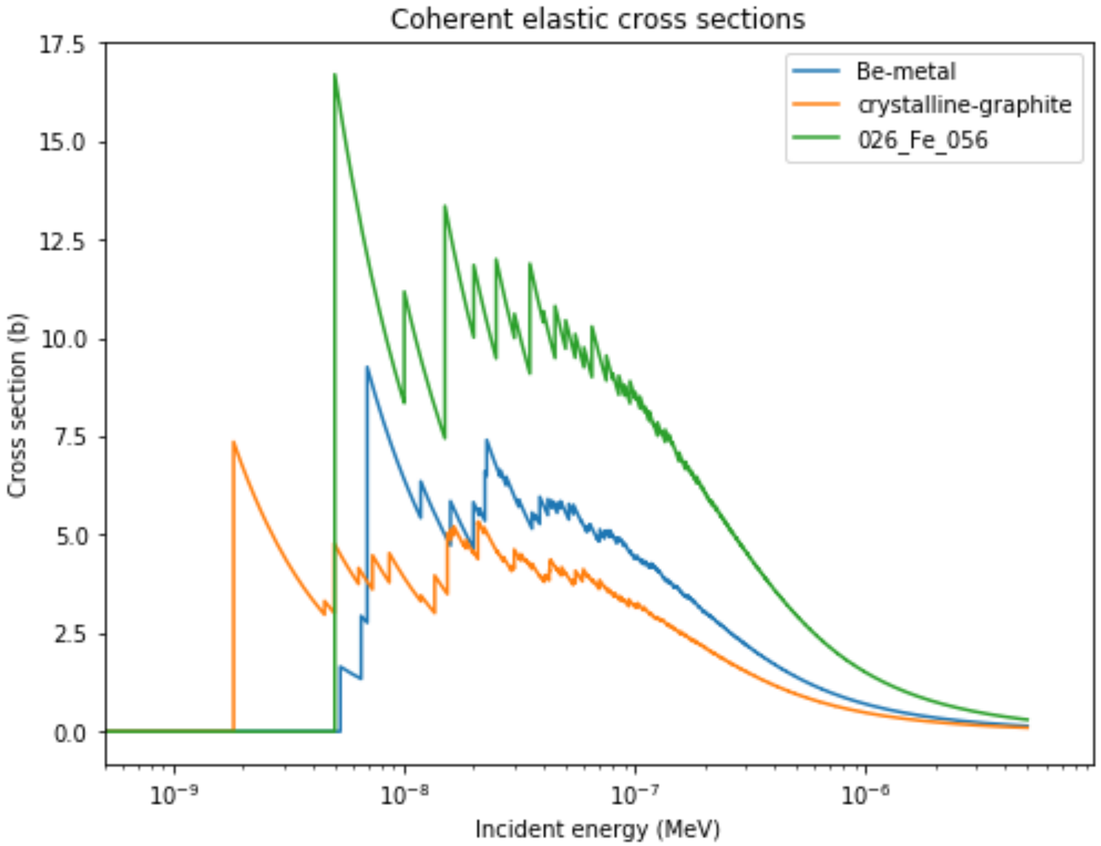
Coherent elastic: bulk scattering off crystalline materials

$$\frac{d^2\sigma}{dE'\,d\Omega}(E \to E', \mu, T) = \frac{1}{E}\sum_{i=1}^{E_i<E} s_i(T)\,\delta(\mu-\mu_i)\,\delta(E-E')/2\pi$$

where

$$\mu_i = 1 - \frac{2E_i}{E}$$

- Outgoing angular distribution consists of delta functions at various μ_i
- TODO: sample angles directly using $s_i(T)$
  - Requires some work in GIDI+

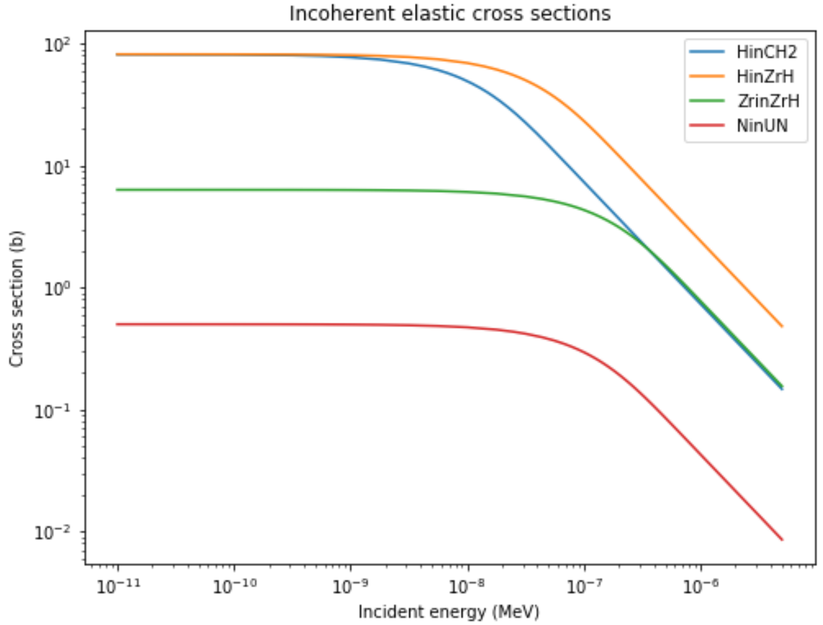


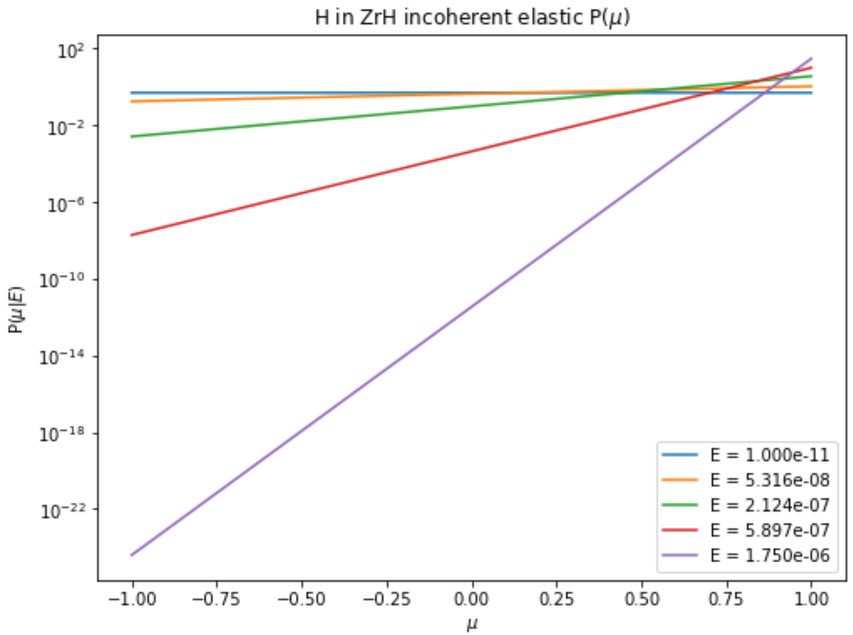
C. Mattoon IAEA CM on Data Processing, Oct. 2021

Incoherent elastic: bulk scattering off partially ordered materials

$$\frac{d^2\sigma}{dE'\,d\Omega}(E \to E', \mu, T) = \frac{\sigma_b}{4\pi}\, e^{-2EW'(T)(1-\mu)}\ \delta(E - E')$$

where σ_b and W'(T) are tabulated



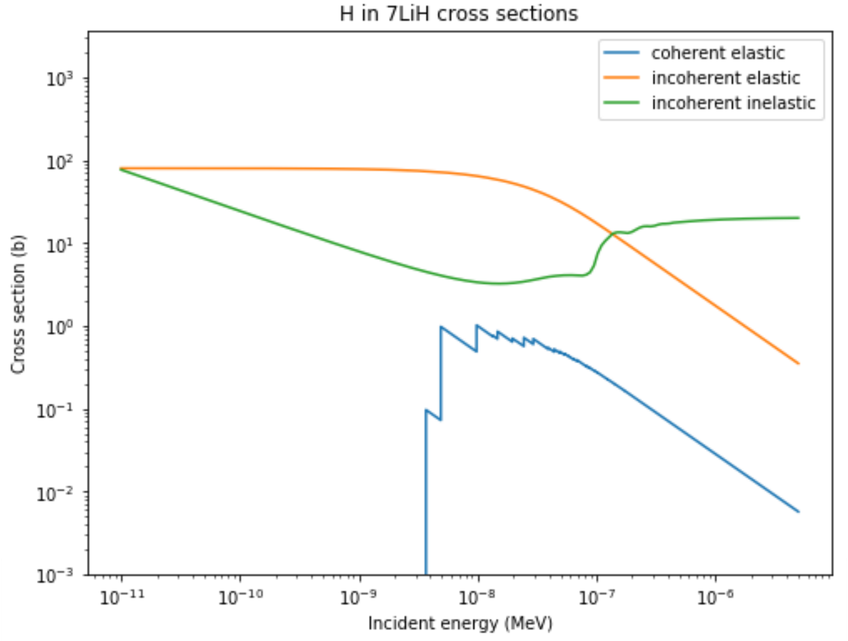


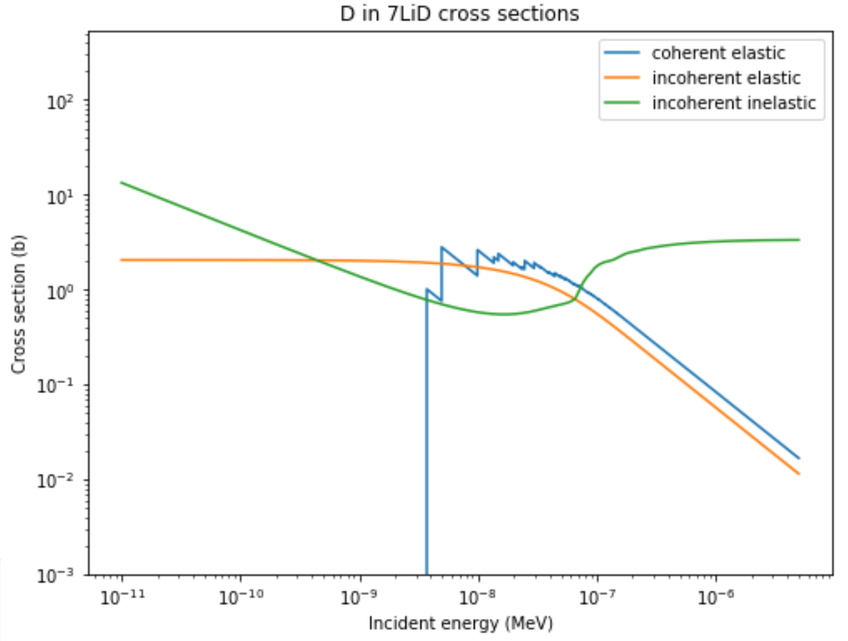
Again, seems more efficient to use W'(T) to sample directly… TBD

C. Mattoon IAEA CM on Data Processing, Oct. 2021

GNDS easily handles new LTHR=3 (mixed elastic) format proposed by M. Zerkle

- Some materials require both coherent elastic and incoherent elastic (plus inelastic) to properly represent thermal scattering region.
- Handled in GNDS simply by adding another ***reaction*** node for the new elastic term
- Example files for ^{7}LiH and ^{7}LiD were translated to GNDS and processed with FUDGE
  - Results can be translated to ENDL, ACE coming soon once we check latest format update…





Incoherent inelastic is trickier, often requiring extrapolation beyond tabulated $S_{\alpha\beta}$ grid especially at forward angles.

$$\frac{d^2\sigma}{d\Omega\, dE'}(E \to E', \mu, T) = \sum_{n=0}^{\mathrm{NS}} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S_n(\alpha, \beta, T)$$

$$\alpha = \left[E' + E - 2\mu\sqrt{EE'}\right] \; /A_0 kT$$

$$\beta = (E' - E)/kT$$

- A_0, M_n, σ_{bn}, $S_n(\alpha,\beta,T)$ are tabulated
- α,β grids in many evaluations aren't sufficient for spanning all (E, E', μ) of interest
  - Short collision time (SCT) approximation is appropriate for large α,β but generally not as α approaches 0
  - Extrapolation required for small α, but appears to be handled differently by processing codes
    - Especially relevant for forward scattering where E' ≈ E

C. Mattoon IAEA CM on Data Processing, Oct. 2021

GNDS-2.0 Highlights

- **xsdir-like functionality:**
  `map` file and `checksum` support
- **Documentation markup:**
  supports all metadata needed for DataCite.org DOI assignment
- **Ground-up rewrite of TNSL**
  - In collaboration with SG-42,48
  - Mixed elastic scattering
  - TNSL covariance
- **Cleanups and bug fixes**
- **Full support for ENDF-6 data**
- **Met all SG-38 requirements**

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        standardTarget="H1" standardEvaluation="ENDF/B-8.0"/>
  <protare projectile="n" target="O16" evaluation="ENDF/B-7.1"
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</map>
```
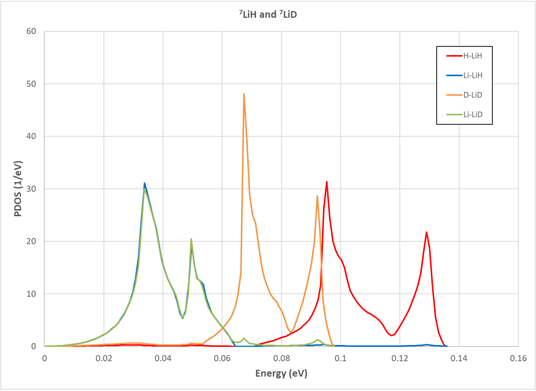
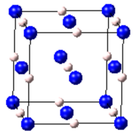
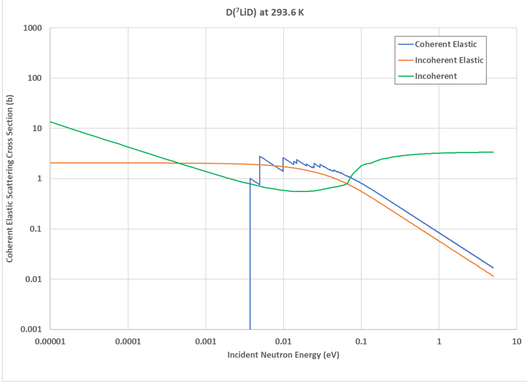





LiH unit cell
(4.0831 Å for LiH,
4.0684 Å for LiD)



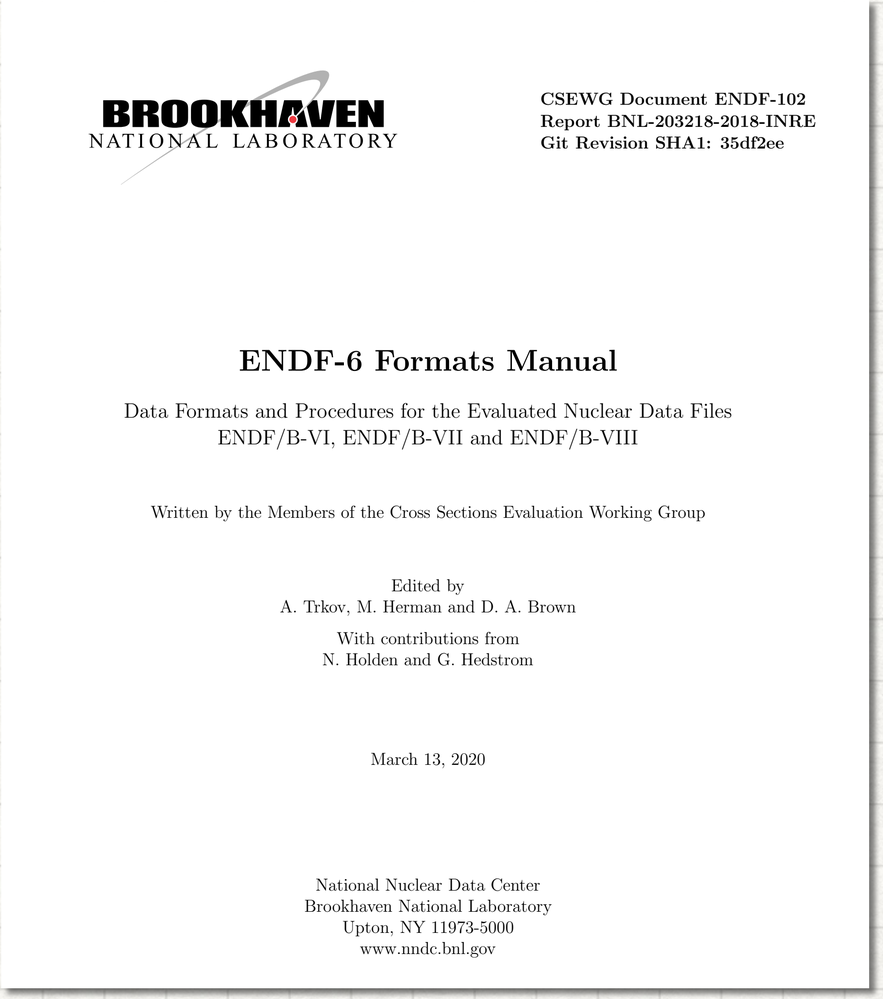
SPECIFICATIONS VS. REQUIREMENTS VS. ENDF-6

D. Brown (NNDC, BNL)

D.Brown 2021 WPEC EG-GNDS meeting

GNDS VS. ENDF-6

- All MF/MT's in ENDF-6 manual have GNDS analogs
- All low level formats in ENDF-6 are either obsolete or have GNDS analogs
- Developed 4 page summary showing connection between ENDF-6 and GNDS.
  - Suggest making it an appendix to specifications
- TO DO: detailed (LIP/LAW/ whatever level) comparison between formats



BROOKHAVEN NATIONAL LABORATORY

CSEWG Document ENDF-102
Report BNL-203218-2018-INRE
Git Revision SHA1: 35df2ee

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
A. Trkov, M. Herman and D. A. Brown

With contributions from
N. Holden and G. Hedstrom

March 13, 2020

National Nuclear Data Center
Brookhaven National Laboratory
Upton, NY 11973-5000
www.nndc.bnl.gov

GNDS VS. SG-38 REQUIREMENTS

- Approved map/library/xsdir/etc file markup
- Proper treatment of EOS in TNSL data
- Some elements of atomic data
- Improved FPY markup
- Processed data types
- Radiation damage
- dE/dx
- Resonance things: Brune transform, CP RRR
- **Improved TNSL markup (see proposal/TNSL)**
- **Improved documentation markup (see proposal/documentation)**
- **Support for the sandwich formula (see proposal/sandwichProduct)**
- **TO DO: detailed comparison between format and each requirement sub-bullet**

Generally unwise to force format discussion until we see what evaluators can provide & see what users need

We’ll be editing the specifications for a while

Required for final preparation of document

- Passive voice is required in all OECD publications
- British, not American spelling
- Discussion point -> Tracker conversion
- Many, many branches
- Many unclear formulations remain (e.g. interpolation)
- Update appendix with changelist

Implementation status? See talks from LLNL, LANL, & ORNL

What's next

- **Expect major format changes post-GNDS-2.0:**
  - Synchronize nuclear structure formats with ENSDF as part of ENSDF modernization
  - Revamp uncertainty/covariance to make more ML friendly
  - Atomic data additions
  - FPY formats per FIRE collaboration recommendations

- **ENDF to GNDS transition:**
  - ENDF/B-VIII.0 released in GNDS-1.9
  - ENDF/B-VIII.1, JEFF-4, TENDL to be released in GNDS-2.0
  - Expect at least next release to be in both ENDF-6 and GNDS formats
  - Transition is slow; we must walk together and we can only go as fast as the slowest among us

I am stepping down as EG GNDS chair once 2.0 is out the door